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Engineering Cyclic Tetrapeptides Containing Chimeric Amino Acids as Preferred Reverse-Turn Scaffolds
Che, Y.; Marshall, G. R.
J. Med. Chem.; **(Article); 2006**; *49*(1); 111-124. DOI: 10.1021/jm0507072

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Neopetrosiamides, Peptides from the Marine Sponge *Neopetrosia* sp. That Inhibit Amoeboid Invasion by Human Tumor Cells
Williams, D. E.; Austin, P.; Diaz-Marrero, A. R.; Soest, R. V.; Matainaho, T.; Roskelley, C. D.; Roberge, M.; Andersen, R. J.
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Deazapurine Solid-Phase Synthesis: Construction of 3-Substituted Pyrrolo[3,2-*d*]pyrimidine-6-carboxylates on Cross-Linked Polystyrene Bearing a Cysteamine Linker
Rombouts, F. J. R.; Fridkin, G.; Lubell, W. D.
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Asymmetric Synthesis of 3-Substituted Proline Chimeras Bearing Polar Side Chains of Proteinogenic Amino Acids
Quancard, J.; Labonne, A.; Jacquot, Y.; Chassaing, G.; Lavielle, S.; Karoyan, P.
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Virtually Complete Control of Simple and Face Diastereoselectivity in the Michael Addition Reactions between Achiral Equivalents of a Nucleophilic Glycine and (*S*)- or (*R*)-3-(*E*-Enoyl)-4-phenyl-1,3-oxazolidin-2-ones: Practical Method for Preparation of β-Substituted Pyroglutamic Acids and Prolines
Soloshonok, V. A.; Ueki, H.; Tiwari, R.; Cai, C.; Hruby, V. J.
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Determinants of Corticotropin Releasing Factor. Receptor Selectivity of Corticotropin Releasing Factor Related Peptides

Mazur, A. W.; Wang, F.; Tscheiner, M.; Donnelly, E.; Isfort, R. J.

J. Med. Chem.; **(Article); 2004**; *47*(13); 3450-3454. DOI: 10.1021/jm049883l

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Sugase, K.; Horikawa, M.; Sugiyama, M.; Ishiguro, M.

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Monitoring the Early Steps of Unfolding of Dicalcium and Mono-Ce^{3+}-Substituted Forms of P43M Calbindin D_{9k}†

Jimenez, B.; Poggi, L.; Piccioli, M.

Biochemistry; **(Article); 2003**; *42*(44); 13066-13073. DOI: 10.1021/bi034638+

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Amino-Zinc-Enolate Carbometalation Reactions: Application to Ring Closure of Terminally Substituted Olefin for the Asymmetric Synthesis of *cis*- and *trans*-3-Prolinoleucine

Karoyan, P.; Chassaing, G.; Quancard, J.; Vaissermann, J.

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Krow, G. R.; Herzon, S. B.; Lin, G.; Qiu, F.; Sonnet, P. E.

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Comparative Assessment of the Ligand and Metal Ion Binding Properties of Integrins $\alpha 9\beta 1$ and $\alpha 4\beta 1$

Pepinsky, R. B.; Mumford, R. A.; Chen, L. L.; Leone, D.; Amo, S. E.; Riper, G. V.; Whitty, A.; Dolinski, B.; Lobb, R. R.; Dean, D. C.; Chang, L. L.; Raab, C. E.; Si, Q.; Hagmann, W. K.; Lingham, R. B.
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The Rearrangement Route to 3-CH_2X-2-azabicyclo[2.1.1]hexanes. Substituent Control of Neighboring Group Participation
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High Selectivity from Configurational Match/Mismatch in Carbon-Hydrogen Insertion Reactions of Steroidal Diazoacetates Catalyzed by Chiral Dirhodium(II) Carboxamidates
Doyle, M. P.; Davies, S. B.; May, E. J.
J. Org. Chem.; **(Article); 2001**; *66*(24); 8112-8119. DOI: 10.1021/jo015932f

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Synthesis of Conformationally Constrained Arginine and Ornithine Analogues Based on the 3-Substituted Pyrrolidine Framework
Mamai, A.; Hughes, N. E.; Wurthmann, A.; Madalengoitia, J. S.
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Peptide and Peptide Mimetic Inhibitors of Antigen Presentation by HLA-DR Class II MHC Molecules. Design, Structure-Activity Relationships, and X-ray Crystal Structures
Bolin, D. R.; Swain, A. L.; Sarabu, R.; Berthel, S. J.; Gillespie, P.; Huby, N. J. S.; Makofske, R.; Orzechowski, L.; Perrotta, A.; Toth, K.; Cooper, J. P.; Jiang, N.; Falcioni, F.; Campbell, R.; Cox, D.; Gaizband, D.; Belunis, C. J.; Vidovic, D.; Ito, K.; Crowther, R.; Kammlott, U.; Zhang, X.; Palermo, R.; Weber, D.; Guenot, J.; Nagy, Z.; Olson, G. L.
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Conformationally Constrained Substance P Analogues: The Total Synthesis of a Constrained Peptidomimetic for the Phe^7-Phe^8 Region
Tong, Y.; Fobian, Y. M.; Wu, M.; Boyd, N. D.; Moeller, K. D.
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Total Synthesis of Gypsetin, Deoxybrevianamide E, Brevianamide E, and Tryprostatin B: Novel Constructions of 2,3-Disubstituted Indoles
Schkeryantz, J. M.; Woo, J. C. G.; Siliphaivanh, P.; Depew, K. M.; Danishefsky, S. J.
J. Am. Chem. Soc.; **(Article); 1999**; *121*(51); 11964-11975. DOI: 10.1021/ja9925249

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Stereoselective Reactions of *N*-(9-Phenylfluoren-9-yl)-4-oxoproline Enolates. An Expedient Route for the Preparation of Conformationally Restricted Amino Acid Analogues
Blanco, M.-J.; Paleo, M. R.; Penide, C.; Sardina, F. J.
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Synthesis and Serotonergic Activity of 3-[2-(Pyrrolidin-1-yl)ethyl]indoles: Potent Agonists for the h5-HT_{1D} Receptor with High Selectivity over the h5-HT_{1B} Receptor
Sternfeld, F.; Guiblin, A. R.; Jelley, R. A.; Matassa, V. G.; Reeve, A. J.; Hunt, P. A.; Beer, M. S.; Heald, A.; Stanton, J. A.; Sohal, B.; Watt, A. P.; Street, L. J.
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Design of Peptidomimetics That Inhibit the Association of Phosphatidylinositol 3-Kinase with Platelet-Derived Growth Factor-β Receptor and Possess Cellular Activity

Eaton, S. R.; Cody, W. L.; Doherty, A. M.; Holland, D. R.; Panek, R. L.; Lu, G. H.; Dahring, T. K.; Rose, D. R.
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Stereoselective Synthesis of Tilivalline[1]
Nagasaka, T.; Koseki, Y.
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2-Nitrophenylcarbamoyl-(*S*)-prolyl-(*S*)-3-(2-naphthyl)alanyl-*N*-benzyl-*N*- methylamide (SDZ NKT 343), a Potent Human NK_1 Tachykinin Receptor Antagonist with Good Oral Analgesic Activity in Chronic Pain Models
Walpole, C.; Ko, S. Y.; Brown, M.; Beattie, D.; Campbell, E.; Dickenson, F.; Ewan, S.; Hughes, G. A.; Lemaire, M.; Lerpiniere, J.; Patel, S.; Urban, L.
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Tandem Asymmetric Cyclopropanation/Cope Rearrangement. A Highly Diastereoselective and Enantioselective Method for the Construction of 1,4-Cycloheptadienes
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A Novel Stereodivergent Synthesis of Optically Pure *cis*- and *trans*-3-Substituted Proline Derivatives
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Potent α4β1 Peptide Antagonists as Potential Anti-Inflammatory Agents

Jackson, D. Y.; Quan, C.; Artis, D. R.; Rawson, T.; Blackburn, B.; Struble, M.; Fitzgerald, G.; Chan, K.; Mullins, S.; Burnier, J. P.; Fairbrother, W. J.; Clark, K.; Berisini, M.; Chui, H.; Renz, M.; Jones, S.; Fong, S.
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Rodriguez, A. D.; Cobar, O. M.; Padilla, O. L.
J. Nat. Prod.; **(Note); 1997**; *60*(9); 915-917. DOI: 10.1021/np970215v

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Enantiodivergent Chemoenzymatic Synthesis of (*R*)- and (*S*)-β-Proline in High Optical Purity

Mazzini, C.; Lebreton, J.; Alphand, V.; Furstoss, R.
J. Org. Chem.; **(Note); 1997**; *62*(15); 5215-5218. DOI: 10.1021/jo9701905

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Sasaki, N. A.; Dockner, M.; Chiaroni, A.; Riche, C.; Potier, P.
J. Org. Chem.; **(Note); 1997**; *62*(3); 765-770. DOI: 10.1021/jo961790r

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Mauger, A. B.
J. Nat. Prod.; **(Review); 1996**; *59*(12); 1205-1211. DOI: 10.1021/np9603479

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Total Synthesis of Tryprostatin B: Generation of a Nucleophilic Prenylating Species from a Prenylstannane

Depew, K. M.; Danishefsky, S. J.; Rosen, N.; Sepp-Lorenzino, L.
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Scott E. Denmark, Lawrence R. Marcin
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Development of a Model for the .delta. Opioid Receptor Pharmacophore. 1. Conformationally Restricted Tyr1 Replacements in the Cyclic .delta. Receptor Selective Tetrapeptide Tyr-c[D-Cys-Phe-D-Pen]OH (JOM-13)
Henry I. Mosberg, Andrei L. Lomize, Chenguang Wang, Heather Kroona, Deborah L. Heyl, Katarzyna Sobczyk-Kojiro, Wenli Ma, Carol Mousigian, Frank Porreca
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Wayne J. Brouillette, Vladimir P. Jestkov, Milton L. Brown, M. Shamim Akhtar, Timothy M. DeLorey, George B. Brown
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Design and Synthesis of Side-Chain Conformationally Restricted Phenylalanines and Their Use for Structure-Activity Studies on Tachykinin NK-1 Receptor
Hubert Josien, Solange Lavielle, Alie Brunissen, Monique Saffroy, Yvette Torrens, Jean-Claude Beaujouan, Jacques Glowinski, Gerard Chassaing
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A conformational study by proton NMR of a cyclic pentapeptide antagonist of endothelin
Murray Coles, Victoria Sowemimo, Denis Scanlon, Sharon L. A. Munro, David J. Craik
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A [3+2] cycloaddition and [4+3] cycloaddition approach to N-heterocycles via palladium-catalyzed TMM reactions with imines
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Synthesis and biological activity of CCK heptapeptide analogs. Effects of conformational constraints and

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Mark W. Holladay, Michael J. Bennett, Michael D. Tufano, C. W. Lin, Karen E. Asin, David G. Witte, Thomas R. Miller, Bruce R. Bianchi, A. L. Nikkel, et al.
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trans-3-n-propyl-L-proline is a highly favorable, conformationally restricted replacement for methionine in the C-terminal tetrapeptide of cholecystokinin. Stereoselective synthesis of 3-allyl- and 3-n-propyl-L-proline derivatives from 4-hydroxy-L-proline
Mark W. Holladay, Chun Wei Lin, Catherine S. May, David S. Garvey, David G. Witte, Thomas R. Miller, Caroline A. W. Wolfram, Alex M. Nadzan
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Electrophilic olefin heterocyclization in organic synthesis. Highly stereoselective synthesis of trans 3,5-disubstituted pyrrolidin-2-ones by iodolactamization via homoallylic asymmetric induction
Hiroki Takahata, Tamotsu Takamatsu, Yinshan Chen, Naoki Ohkubo, Takao Yamazaki, Takefumi Momose, Tadamasa Date
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Conformationally constrained amino acids. Synthesis and optical resolution of 3-substituted proline derivatives
John Y. L. Chung, James T. Wasicak, William A. Arnold, Catherine S. May, Alex M. Nadzan, Mark W. Holladay
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Synthesis of 4-substituted prolines as conformationally constrained amino acid analogs
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Potent, long-acting luteinizing hormone releasing hormone antagonists containing new synthetic amino acids: N,N'-dialkyl-D-homoarginines
John J. Nestor, , Jr. Ram Tahilramani, Teresa L. Ho, Georgia I. McRae, Brian H. Vickery
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J. Eric Nordlander, Mark J. Payne, F. George Njoroge, Michael A. Balk, George D. Laikos, Vasanth M. Vishwanath
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Synthesis of dihydromauritine A, a reduced cyclopeptide alkaloid
Ruth F. Nutt, Kau Ming Chen, Madeleine M. Joullie
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Antihypertensive agents: angiotensin converting enzyme inhibitors. 1-[3-(Acylthio)-3-aroylpropionyl]-L-prolines
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Pyridazinones. 2. Synthesis and antisecretory and antiulcer activities of thiourea and 2-cyanoguanidine derivatives
Toshihiro Yamada, Youichi Nobuhara, Hiroshi Shimamura, Yoshitsugu Tsukamoto, Kazuo Yoshihara, Azuma Yamaguchi, Masahiko Ohki

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Synthesis and stereochemistry of 3-hydroxy-5-methylproline, a new naturally occurring imino acid
Anthony B. Mauger, Oswald A. Stuart, Edward Katz, Kaarin T. Mason
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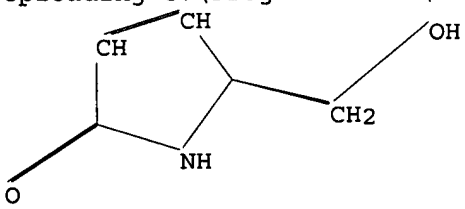

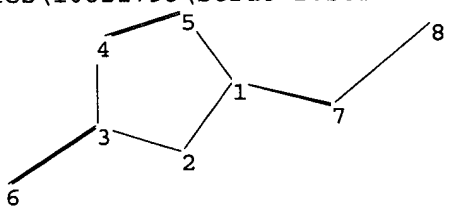


```
chain nodes :
6  7  8
ring nodes :
1  2  3  4  5
chain bonds :
1-7  3-6  7-8
ring bonds :
1-2  1-5  2-3  3-4  4-5
exact/norm bonds :
```

```
1-2  1-5  2-3  3-4  3-6  4-5
exact bonds :
1-7  7-8


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:CLASS  7:CLASS  8:CLASS

Stereo Bonds:

7-1 (Single Wedge).


Stereo Chiral Centers:

1    (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 1

L1      STRUCTURE UPLOADED

=> l1
SAMPLE SEARCH INITIATED 11:19:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     2128 TO ITERATE

 94.0% PROCESSED     2000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        39793 TO    45327
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> l1 full
FULL SEARCH INITIATED 11:19:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    43131 TO ITERATE

100.0% PROCESSED    43131 ITERATIONS                                  1 ANSWERS
SEARCH TIME: 00.00.01

L3            1 SEA SSS FUL L1

=> d hitstr
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats.  The predefined substance formats
are:  (RN = CAS Registry Number)

REG     - RN
SAM     - Index Name, MF, and structure - no RN
FIDE    - All substance data, except sequence data
IDE     - FIDE, but only 50 names
SQIDE   - IDE, plus sequence data
SQIDE3  - Same as SQIDE, but 3-letter amino acid codes are used
SQD     - Protein sequence data, includes RN
```

SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):rn sam
'SAM' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties

PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

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CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
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IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):d rn sam
'SAM' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'D' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats

must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

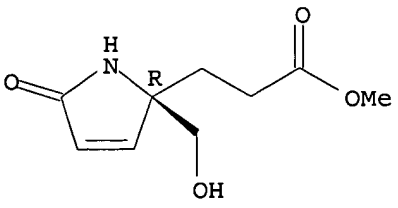
The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):sam

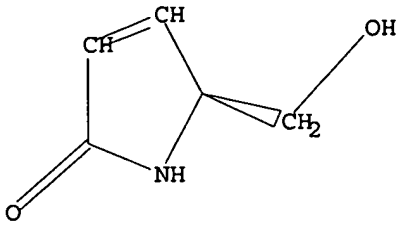
L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
IN 1H-Pyrrole-2-propanoic acid, 2,5-dihydro-2-(hydroxymethyl)-5-oxo-, methyl ester, (R)- (9CI)
MF C9 H13 N O4

Absolute stereochemistry. Rotation (-).



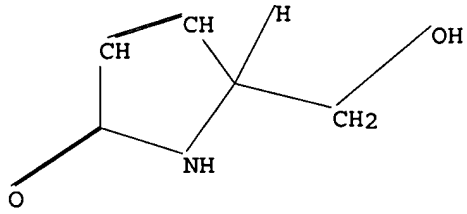
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

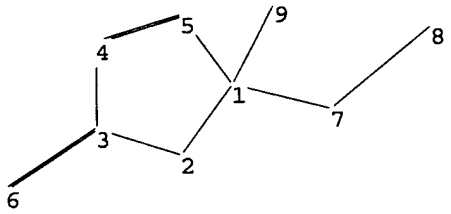
=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=>
Uploading C:\Program Files\Stnexp\Queries\10821793\Struc 3.str



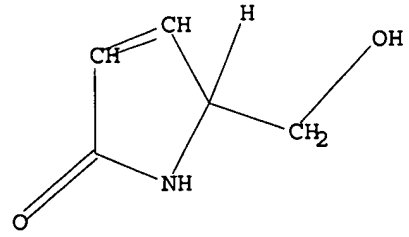


chain nodes :
6 7 8 9
ring nodes :
1 2 3 4 5
chain bonds :
1-7 1-9 3-6 7-8
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-6 4-5
exact bonds :
1-7 1-9 7-8

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> l4
SAMPLE SEARCH INITIATED 11:22:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     2128 TO ITERATE

 94.0% PROCESSED     2000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        39793 TO    45327
PROJECTED ANSWERS:               0 TO        0

L5             0 SEA SSS SAM L4

=> l4 full
FULL SEARCH INITIATED 11:22:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    43131 TO ITERATE

100.0% PROCESSED    43131 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

L6             0 SEA SSS FUL L4

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   336.58     336.79

STN INTERNATIONAL LOGOFF AT 11:22:44 ON 05 JAN 2006
```